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13. ABSTRACT (Maximum 200 words)

A focal point of the research conducted during the contract period has been TR8, TR11, TR17, TR19, and TR26. Microgravity combustion was a secondary focal point during the later period, described in TR14, TR15, TR22, TRR24, TR28, and TR29. A total of 29 technical reports was generated of which, so far, 17 has appeared in print. The titles and abstracts of these reports may be found below. The PI has given a large number of talks on contract related work, many of them by invitation and at no expense to the contract. Those of the past 2 years are listed below. Other recognition is also listed.

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THE STRUCTURE AND STABILITY OF THREE-DIMENSIONAL DETONATION WAVES

Summary

A focal point of the research conducted during the contract period has been the nonlinear behavior of detonation waves. This work is described in TR2, TR4, TR8, TR11, TR16, TR17, TR19, and TR26. Microgravity combustion was a secondary focal point during the later period, described in TR14, TR15, TR22, TR24, TR28, and TR29. A total of 29 technical reports was generated of which, so far, 17 have appeared in print. The titles and abstracts of these reports may be found below.

The PI has given a large number of talks on contract related work, many of them by invitation and at no expense to the contract. Those of the past 2 years are listed below. Other recognition is also listed.

Technical Reports.

Appended is a list of all Technical Reports (including Abstracts) generated since May 1 1986. Copies have been sent to Dr. A. Nachman.

Recognition

1986 PI elected a fellow of the American Physical Society

1988 PI awarded a fellowship from the Japanese Society for the Promotion of Science

1990 PI awarded a John Simon Guggenheim fellowship

Talks at Meetings, Seminars etc. since May 1, 1988

May 1988. Talks at a number of Japanese Universities (Tsukuba, Tokyo, Nagoya, Kyoto, Sendae, Sapporo) during an extended visit as a guest of the Japanese government (JSPS Fellow). In particular, I gave a series of talks on detonation theory at the University of Nagoya.

May 1988. BAIL V, Shanghai - see TR20.

July 1988. University of Bordeaux.

July 1988. Invited plenary lecture at the 1st National Fluid Dynamics Congress, Cincinnati.

August 1988. 22nd Symposium (International) on Combustion, Seattle, see TR9.

August 1988. International Workshop on Mathematics in Combustion, Vancouver, B.C.

August 1988. International Congress on Theoretical and Applied Mechanics (Congress IUTAM 88), Grenoble.

November 1988. 41st Annual Meeting of the Fluid Dynamics Division of the American Physical Society.

January 1989. Pan American Congress on Applied Mechanics (see TR 21).

January 1989. Poster display at the NASA Lewis microgravity combustion workshop.

February 1989. Invited lecture at the program 'Problemes Non Lineares Appliques', organized by INRIA, Rocquencourt (see TR 22).

March 1989. Invited lectures at the program 'Fluid Dynamical Aspects of Combustion Theory', organized by CNR, Rome.

April 1989. University of Buffalo.

May 1989. University of Madrid.

May 1989. University of Marseille.

May 1989. Third International Conference on Numerical Combustion, Antibes.

July 1989 International Conference on the Dynamics of Explosive and Reactive Systems.

October 1989 Invited lecture at a combustion workshop sponsored by NASA ICASE.

October 1989 Seminar, ENS, Lyon, France

November 1989 Invited lecture at the 'Mathematics in Chemistry Conference' College Station, Texas

November 1989 Invited lecture at the IMA workshop on 'Dynamical Issues in Combustion Theory', Minneapolis.

November 1989 42nd Annual Meeting of the Fluid Dynamics Division of the American Physical Society

March 1990 Invited lecture at a combustion workshop in Tsukuba, Japan.

Visitors.

In October 1988, Dr.Claudine Schmidt-Laine visited the University of Illinois for 2 weeks, at NATO expense, to collaborate on contract problems.

In February 1989, Dr. William Dold visited for 4 weeks to collaborate on contract problems.

Appendix.

Technical Reports produced since May 1, 1986.

TR1. 'The infinite candle and its stability - a paradigm for flickering diffusion flames'. J. Buckmaster and N. Peters.
Proceedings of the 21st (International) Symposium on Combustion, 1986, published by the Combustion Institute, Pittsburgh, Pa., p. 1829.
TR2. 'The effect of structure on the stability of detonations. I. The role of the induction zone'. J.Buckmaster and G.S.S.Ludford.
Proceedings of the 21st (International) Symposium on Combustion, 1986, published by the Combustion Institute, Pittsburgh, Pa., p. 1669.

TR3. 'Extinction behavior of tubular flames for small Lewis number'.
T.Takeno, S.Ishizuka, M.Nishioka, and J.D.Buckmaster.
Springer Series in Chemical Physics 47, 1987, editors J. Warnantz and W. Jager, Springer-Verlag, p. 302-309

TR4. 'Pressure transients and the genesis of transverse shocks in unstable detonations'. J.Buckmaster.
Combustion Science and Technology, 1988, vol.61, p.1.

TR5. 'Mathematical modeling in the age of computing: is it redundant?'.
J.Buckmaster.
Invited paper in Mathematical Modeling in Combustion and Related Topics, eds. C.M. Brauner and C.Schmidt-Laine. NATO ASI Series, Series E: Applied Sciences No.140, published by Martinus Nijhoff, Boston, 1988, p.29.

TR6. 'On the abrupt extinction of premixed flames with Lewis numbers less than one'. D.Mikolaitis.
Combustion and Flame.

TR7. 'Convection effects and the stability of hydrogen flame bubbles'.
J.Buckmaster, R.E.Johnson, and S.Weeratunga.
In Mathematical Modeling in Combustion Science. eds. J.D.Buckmaster and T.Takeno, Springer-Verlag, New York, Lecture Notes in Physics, vol.299. p.112.

TR8. 'One-dimensional detonation stability- the spectrum for infinite activation energy'. J.Buckmaster and J.Neves.
Physics of Fluids, vol.31, No.12, 1988, p.3571.

TR9. 'Anomalous Lewis number effects in tribrachial flames'. J.Buckmaster and M.Matalon.
Proceedings of the 22nd (International) Symposium on Combustion, 1988, published by the Combustion Institute, Pittsburgh, p. 1527-1535.

TR10. 'The flow field of hydrogen flame bubbles or caps and its stabilizing influence', re-titled 'A flame-bubble analogue and its stability'. S.Weeratunga, J.Buckmaster and R.E.Johnson.
Combustion and Flame, 79, 1990, p. 100-109.

TR11. 'A theory for triple point spacing in overdriven detonation waves'. J.Buckmaster.
Combustion and Flame, 77, 1989, p. 219-228.

TR12. 'Effects of a slow gas-phase reaction on the L* instability in solid propellant rockets: Part I, Linear stability'. H.I. Lee and J.Buckmaster.

TR13. 'Effects of a slow gas-phase reaction on the L* instability in solid propellant rockets: Part II, Nonlinear study'. H.I. Lee and J.Buckmaster.

TR14. 'The effects of radiation on flame-balls at zero gravity', re-titled 'The structure and stability of non-adiabatic flame-balls'. J.Buckmaster, G.Joulin, and P.Ronney.
Combustion and Flame, 79, 1990 p. 381-392.

TR15. 'Radial propagation of premixed flames and $\sqrt{t}$ behavior'. J.Buckmaster and G.Joulin.
Combustion and Flame, 78, 1989, p. 275-286.

TR16. 'Flow refraction by an uncoupled shock and reaction front'. J.Buckmaster and C.J. Lee.
AIAA Journal, in press (1990).

TR17. 'Pressure spot formation in unstable detonation waves'. C.Schmidt, W.Dold, and J.Buckmaster.
Proceedings of the Third International Conference on Numerical Combustion, Antibes, France, May 23-26, 1989. Published as Lecture Notes in Physics 351, edited by A. Dernieux and B. Larrouturou, Springer-Verlag, 1989, p. 428-439.

TR18 'A natural convection problem arising from the study of flame-bubbles'. S.Weeratunga, J.Buckmaster, and R.E.Johnson.
Applied Mechanics Reviews, Part 2 of Vol. 42, No. 11, November 1989.

TR19. 'The structural stability of oblique detonation waves'. J.Buckmaster, Combustion Science and Technology, in press (1990).

TR20. Unexpected Lewis number effects in tribrachial flames'. J.Buckmaster and M.Matalon.

Invited contribution to BAIL V, Proceedings of the Fifth International Conference on Boundary and Interior Layers - Computational and Asymptotic Methods, 20-24 June 1988, Shanghai, China, p.1. (A summary of TR9).

TR21. 'Downstream boundary conditions in a natural convection problem'. S.Weeratunga, J.Buckmaster, and R.E.Johnson.
Proceedings of the First Pan American Congress of Applied Mechanics (PACAM), Rio de Janeiro, Brazil, Jan.3-6, 1989, p.384. No publisher identified. By invitation, an extended version is reported in TR18.

TR22. 'Modeling of μ_g ignition experiments'. J.Buckmaster, G.Joulin and P.Ronney.
Invited contribution to the Proceedings of the meeting, Problemes non linearies appliques, Rocquencourt, France, Feb.27-Mar.3, 1989, in press.

TR23. 'Flame stability', J. Buckmaster.
Proceedings of a combustion workshop held in Hampton, VA., Oct. 4, 1989, sponsored by NASA ICASE. In press.

TR24. 'The structure and stability of non-adiabatic flame-balls, II. Effects of far-field losses'. J. Buckmaster, G. Joulin and P. Ronney.

TR25. 'Linear stability of one-dimensional detonations' G. Namah, C. Brauner, J. Buckmaster, and C. Schmidt-Laine.
Proceedings of the workshop on 'Dynamical Issues in Combustion Theory' held at the Institute for Mathematics and its Applications, Minnesota, Nov. 13-17, 1989. To be published in the series IMA Volumes in Mathematics and its Applications, Springer-Verlag.

TR26. 'On an evolution equation arising in detonation theory' C. Brauner, J. Buckmaster, J. W. Dold, and C. Schmidt-Laine.
To appear in Fluid Dynamic Aspects of Combustion Theory.

Longmons, the Proceedings of a year long special program held at the Institute per le Applicazioni del Calcolo 'Mauro Picone', Rome.

TR27. 'Mathematical Topics in Combustion' J. Buckmaster

Proceedings of the 'Mathematics in Chemistry Conference' held in College Station, Texas, Nov. 8-10, 1989. To be published in a special issue of the Journal of Chemometrics and the Intelligent Laboratory Systems.

TR28. 'Flame-balls stabilized by suspension in fluid with a steady linear ambient velocity distribution. J. Buckmaster and G. Joulin.

TR29. 'The structure and stability of flame-balls: a NEF analysis' C. J. Lee and J. Buckmaster.

Abstracts of Technical Reports.

TR1. Diffusion flames on tube burners flicker at approximately 11 Hz, a frequency that is insensitive to the flow rate, choice of gases, or burner size. We suggest that this is due to the Kelvin-Helmholtz instability of the buoyancy-induced part of the flow-field, an annular region surrounding the forced-convection jet. A model of this flow (the 'infinite candle') permits a stability analysis which predicts a frequency in rough agreement with the experimental value, the best that can be expected in view of the approximations involved.

TR2. The steady structure of detonation waves is easily derived for one-step Arrhenius' kinetics in the limit of infinite activation energy. This paper is concerned with the stability of this solution. An explicit dispersion relation is deduced which predicts unconditional instability. A key physical ingredient which is responsible for the instability is the transient storage of mass, momentum and energy in the chemical induction zone between the lead shock and the region of intense reaction. The length of this zone fluctuates significantly.

TR3. Professor Ishizuka has developed a new combustion configuration for the study of premixed flames, the so-called 'tubular flame'. When the Lewis number is small the flame curvature is very large, and special care must by taken with the asymptotic treatment. This paper addresses that question and obtains results for small Lewis number which can by compared with experimental results.

TR4. TR2 is a linear stability analysis, valid for large activation energy. In this report a nonlinear description is provided of the evolution from a small initial disturbance of the steady unstable detonation wave. This nonlinear development is based on asymptotics valid when the activation energy is large. It describes sharp increases in pressure for the one-dimensional problem, typical of those seen in numerical calculations. During these increases a sonic point is created in the (initially) overdriven detonation wave. For the two-dimensional problem the pressure increase is confined to discrete points distributed along the plane of the wave, and it is suggested that this is the origin of the transverse waves that are seen in practice.

TR5. The text of an invited talk first given at the SIAM Conference on Numerical Combustion, San Francisco, March 1987, this describes three problems in order to refute the notion that mathematical modeling is not necessary in the age of the supercomputer. The three problems are: the lifting of turbulent diffusion flames; hydrogen flame bubbles (TR7); and nonlinear detonation stability (TR4).

TR6. This analyzes the governing equations of reacting low Mach number flows for premixed flame structures in non-uniform flow fields given that the activation temperature of the mixture is large compared to the temperature of the remote reactants. An extinction mechanism is uncovered for flames with Lewis numbers less than one that cannot by found through the use of activation energy asymptotics.

TR7. Hydrogen 'flame-bubbles' are the small flames obtained in very lean hydrogen/air mixtures. Previous estimates of the flame temperature fail to account for convection, and a simple mathematical model is proposed to remedy this. In addition, it is pointed out that convective gradients generated by the buoyancy of the hot wake gases could provide a necessary stabilizing mechanism.

TR8. We provide a description of the spectrum defined by the one-dimensional detonation stability problem in the limit of infinite activation energy. The single eigenvalue identified in TR2 is part of this spectrum, but, in addition, there are an infinite number of discrete eigenvalues whose growth rate is an increasing function of frequency. Convincing speculations on how this spectrum would be modified for finite activation energy, provide useful insights into experimental results for pulsating detonations.

TR9. Flame propagation in mixtures of nonuniform composition often leads to tribrachial flames (three-armed flames - what others have called triple flames) characterized by two premixed branches (fuel-rich and fuel-lean) trailed by a diffusion flame. When the Lewis number =1, the premixed pair forms a C-shaped front, as expected; but for small Lewis numbers the front is S-shaped and it is not clear that the solution is meaningful as an unbounded freely-propagating flame.

TR10. An extension and detailed exposition of some ideas presented in TR7.

TR11. This is similar to the analysis of TR2 except that it examines the behavior of disturbances with smaller wavelengths. The growth rate is a decreasing function of wavenumber and sufficiently short waves are stable. When combined with TR2 these results predict that there is a disturbance wavelength for which the growth rate will be a maximum, and it is suggested that this length is relevant to the initial spacing of the Mach stems that are known to arise in unstable detonations.

TR12. The burning of double-base propellants is often characterized by a dual flame structure in which a normal deflagration is followed by a small Damkohler number flame in which diffusion is negligible. In time-dependent problems (e.g. stability analyses) this second flame may be sufficiently thick that the usual quasi-steady approximation adopted for the gas-phase should be modified. This report describes a linear stability analysis in which the time derivatives are retained in the solid phase (as always) and the second flame, but the combustion field associated with the first flame is quasi-steady.

TR13. See TR12. This describes numerical solutions of the non-linear equations. TR12 and 13 are based on H.Lee's Ph.D. thesis (University of Illinois, College of Engineering, 1988).

TR14. Microgravity experiments in mixtures with small Lewis numbers reveal the possibility of 'flame-balls' - stationary, spherical premixed flames in which the only fluxes are diffusional. In constructing theoretical models of these creatures, a key question is that of stability. In this paper it is shown that

radiative heat losses can stabilize flame-balls. Stationary solutions are described and both 1 and 3 dimensional stability analyses are carried out.

TR15. Microgravity point ignition experiments show that for certain gases the radius of the propagating spherical flame grows like $\sqrt{t}$, where t is the time from initiation. This paper shows how such behavior is predicted from simple model equations valid for mixtures for which Le<1. The analysis proceeds in three distinct stages, corresponding to different time ranges, which we call Zeldovich flames, intermediate flames, and Slowly Varying Flames(SVFs), the latter being classical.

TR16. When a wedge is placed in a hypersonic reacting gas, an attached oblique detonation wave can be generated. Given the nature of the gas and the flow Mach number, there is a maximum permissible wedge angle, defined by the Rankine-Hugoniot equations. Some recent numerical calculations by Fujiwara show, for some conditions, wedge (i.e. flow-deflection) angles larger than those permitted in this way. However, in all such cases, there is a finite angle between the lead shock and the main reaction zone, so that single-front Rankine-Hugoniot conditions are not appropriate. We show that accounting for refraction by two fronts permits larger wedge angles, thus explaining Fujiwara's results.

TR17. The analysis of TR11 is inherently nonlinear, and leads to an evolution equation that describes the location of the lead shock in an unstable detonation wave. Only the linear stability consequences of this equation are examined in TR11, but here we integrate the nonlinear equation numerically. It is shown that, after a finite time, singularities appear in the solution corresponding to the formation of intense pressure spots. It is speculated that these spots will lead to the emergence of transverse shock waves.

TR18. This paper is concerned with the flow-field that will be generated by 'flame-bubbles' (TR7) and is based on S.Weeratunga's Ph.D. thesis (University of Illinois, College of Engineering, 1986). The Navier-Stokes equations for an incompressible, variable density, heat-conducting, buoyant gas are solved numerically, with heat sources distributed in an assigned fashion to represent the flame. The rise speed (i.e. the speed of the flame relative to the far-field) is assigned. The effects on the flow-field of varying the Froude number, Reynolds number, and the strength of the heat sources is explored.

TR19. As noted in TR16, numerical calculations of nominal oblique detonation waves by Fujiwara sometimes lead to a structure in which the shock and the reaction zone are uncoupled in the sense that they drift apart as distance from the wedge axis increases. In this paper it is suggested that this is a structural (spatial) stability problem. Small deviations from a 1 D structure introduced at some distance from the wedge axis will increase as this distance is increased.

TR20. See TR9.

TR21. See TR18.

TR22. This is a summary of TR14 and TR15, together with some additional stability results for flame-balls. Flame-balls have only been observed in mixtures with very small Lewis numbers and it is natural to ask if there is a theoretical reason. Here it is shown that when Le=1, flame balls with heat losses are unconditionally unstable.

TR23. Combustion systems are often unstable and, in technological applications, this can have an adverse effect (damage, for example), a favorable effect (e.g. enhanced burning), or be of no consequence. In some cases the instability arises from interaction between the combustion field and the surrounding apparatus (e.g. singing flames [1], high frequency acoustic instabilities in rocket motors [2]); in other cases the instability is intrinsic to the combustion field. The latter are briefly reviewed here.

TR 24. A theory of spherical premixed flames in which the only transport processes are diffusion and radiation ("flame-balls") is extended to include the effects of heat loss from the far-field (unburned gas). Using matched asymptotic expansions for large activation energy, stationary solutions are constructed and an evolution equation for the radial motion of the flame is derived. Linear stability analyses are performed for both one-dimensional and three-dimensional perturbations. It is shown that when far-field losses are included, the stability properties are qualitatively changed. A smaller range of conditions produces flames that are stable to one-dimensional disturbances and, in some cases, the linear growth rates are found to have imaginary components. Numerical integrations of the evolution equation reveal oscillations (but not limit cycles), in agreement with a bifurcation analysis. The minimum flame-ball radius for which three-dimensional instabilities will occur is shown to depend only on the near-field losses, and becomes arbitrarily large as these losses are reduced.

TR25. We examine the one-dimensional stability of plane detonations characterized by one-step Arrhenius kinetics, using numerical techniques. A pseudo-spectral method, specifically a collocation scheme with Tchebychev polynomials, provides an approximation to the unstable discrete spectrum, in addition to permitting the calculation of stability boundaries in parameter space. We show that behavior predicted by Buckmaster and Neves (Physics of Fluids 31(12) December 1988, p. 3571-6) using activation energy asymptotics, can occur for physically realistic values of the activation energy. That is, the growth rate of the modes (real part of the eigenvalue) can be a monotone function of the frequency (imaginary part). The present work forms part of the Ph.D. thesis of the first author to be submitted to the faculty at the University of Bordeaux.

TR26. Detonation waves are, for the most part, unstable and it is important to understand the origins and consequences of the instability. Since activation energy asymptotics is such a valuable tool in small Mach number combustion, it is natural to try it on the detonation problem, a high Mach number phenomenon, and there have been several attempts of this nature. Some of this work will be reviewed here.

In a certain distinguished limit, an evolution equation can be deduced for the shock displacement, specifically

$$g_t = -\frac{1}{2}(g_y)^2 + \ln\left[\frac{e^{c g_{yy}} - 1}{c g_{yy}}\right], \quad y \in [0, l]$$

$$g_t(0,t) = g_y(l,t) = 0 \; .$$

This equation has been solved numerically and solutions have been found that exhibit singular behavior after a finite time. The stability of the stationary solution $g \equiv 1$ is of interest and a linear analysis provides the qualitative framework. However, a higher order approximation of the invariant manifolds validates the numerics. This describes the nonlinear effects at the saddle point. In the degenerate case $l = l_c = \pi\sqrt{\frac{c}{2}}$ a center-manifold analysis has to be performed.

TR27. A number of mathematical approaches that are currently of interest in theoretical combustion are briefly described. These are: (i) activation energy asymptotics - flame-sheets and hot-spots; (ii) bifurcations and routes to chaos; (iii) turbulent premixed flames - fractals and renormalization ; (iv) reduced chemistry and rate-ratio asymptotics; (v) nonlinear high-frequency acoustics and combustion.

TR28. The ignition of lean H_2/air mixtures under microgravity (μg) conditions can lead to the formation of spherical premixed flames (flame-balls with small Peclet (Pe) and Schmidt (Sc) numbers. A central question concerning these structures is the existence of appropriate stationary stable solutions of the combustion equations. In this paper we examine an individual flame-ball that is suspended in a fluid whose velocity far from the flame is steady and varies linearly in space. Detailed results are obtained for simple shear flows and simple straining flows, both axisymmetric and plane.

Convection enhances the flux of heat from the flame and the flux of mixture to the flame, but because Sc is greater than Pe the relative impact on the former is greater than on the latter. Consequently, there is a net loss of energy from the flame to the far-field, and if large enough this will quench the flame. For values of shear or strain less than the quenching value there are two possible stationary solutions, but one of these is unstable to spherically-symmetric disturbances of the flame-ball. The radius of the other solution is unbounded as Pe and Sc go to zero. Examination of a class of three-dimensional disturbances reveals no additional instability when the energy losses are due only to convection, but sufficiently large flame-balls are unstable when volumetric heat losses from radiation are accounted for. This last result is in agreement with previous results that have been obtained for zero Sc and Pe albeit with an inadequate accounting for the flow field generated by the perturbations.

TR29. We examine the structure and stability of flame-balls in the context of an asymptotic analysis in which $\theta \to \infty$, $(1\text{-}Le) = O\left(\frac{1}{\theta}\right)$, where θ is the activation energy, Le the Lewis number. The heat-loss mechanism necessary for stable solutions is radiation from the burnt gas. For heat losses less than the quenching value there are two stationary solutions, but the one with the smaller radius is always unstable to one-dimensional disturbances. When Le = 1 the large solution is also unstable, but for $Le < Le_c < 1$ where Le_c is a critical value, a portion of the large-solution branch is stable. Sufficiently large solutions are always unstable to three-dimensional disturbances, independent of Le. These results imply that flame-balls can only be generated if Le is sufficiently small; and are consistent with previous results which suggest that the three-dimensional instability is not a Turing instability but is instead a creature of the near-field losses.